TITLE OF THE INVENTION

METHOD AND SYSTEM FOR PREDICTING PROCESS PERFORMANCE USING MATERIAL PROCESSING TOOL AND SENSOR DATA

Cross-reference to Related Applications

[0001]   The present application claims priority to previously filed U.S. Application Serial No. 60/391,965, filed on June 28, 2002. This application is related to U.S. Application Serial No. 60/391,966, filed on June 28, 2002. The entire contents of these applications are incorporated herein by reference.

Field of the Invention

[0002]   The present invention relates to material processing and more particularly to a process performance prediction system and method thereof for predicting process performance including process rate and process uniformity.

Background of the Invention

[0003]   One area of material processing in the semiconductor industry which presents formidable challenges is, for example, the manufacture of integrated circuits (ICs). Demands for increasing the speed of ICs in general, and memory devices in particular, force semiconductor manufacturers to make devices smaller and smaller on the substrate surface. Moreover, in order to reduce fabrication costs, it is necessary to reduce the number of steps (e.g., etch steps, deposition steps, etc.) required to produce an IC structure and, hence, reduce the overall complexity of the IC structure and the fabrication methods thereof. These

demands are further exacerbated by both the reduction in feature size and the increase of substrate size (i.e., 200 mm to 300 mm and greater), which places greater emphasis on critical dimensions (CD), process rate and process uniformity to maximize the yield of superior devices.

[0004]   For example, the precise control of trench depth is critical in the damascene structure process that is utilized for forming IC wiring levels and interconnect structures through inter-level dielectric layers. Usually, an etch stop layer is placed under a dielectric layer in order to protect the underlying layers (devices) from being damaged during over-etching. An etch stop layer generally includes a material that when exposed to the chemistry utilized for etching the dielectric layer has an etch rate less than the dielectric layer etch rate (i.e., the etch chemistry has a high etch selectivity to the dielectric layer relative to the etch stop layer). Furthermore, the etch stop layer provides a barrier for permitting an over-etch step to assure that all features on the substrate are etched to the same depth.

[0005]   However, the etch stop layer complicates the process integration, increases manufacturing cost and decreases device performance. Without an etch stop layer, etch depth can vary depending on etch rate (ER) since fixed-time recipes are used. Since, for example, the etch tool is subject to equipment disturbance, the etch rate can change significantly over maintenance cycles. In order to maintain a constant etch rate, frequent tool qualification and maintenance procedures are required. Therefore, in-situ estimation of the etch rate can determine whether the process chamber is in a normal condition and can provide information to control the etch time so that the etch depth is on target.

Summary of the Invention

[0006]   The present invention provides for a material processing system comprising a

process tool and a process performance prediction system. The process performance

prediction system comprises a plurality of sensors coupled to the process tool to measure tool

data and a controller coupled to the plurality of sensors in order to receive tool data. The

controller is configured to predict the process performance for the process tool using the tool

data.

[0007]   The present invention further provides for a method of constructing a process

performance prediction model for a material processing system comprising the step of

recording tool data for a plurality of observations during a process in a process tool of the

material processing system, where the tool data comprises a plurality of tool data parameters.

The method further comprises the steps of recording process performance data for the

plurality of observations during the process in the process tool of the material processing

system, where the process performance data comprises one or more process performance

parameters, performing a partial least squares analysis using the tool data and the process

performance data, and computing correlation data from the partial least squares analysis.

[0008]   The present invention further advantageously provides a method for predicting

process performance of a material processing system using a process performance prediction

model comprising the steps of preparing a process tool, initiating a process in the process

tool, and recording tool data for at least one observation during the process in the process tool

to form a tool data matrix, where the tool data comprises a plurality of tool data parameters.

The method further comprises the steps of performing a matrix multiplication of the tool data

matrix and a correlation matrix to form a process performance data matrix, where the

correlation matrix comprises the process performance prediction model, and predicting the

process performance of the material processing system from the process performance data matrix.

[0009]   The present invention further advantageously provides a method for detecting a fault in a material processing system using a process performance prediction model. The method comprises the steps of preparing a process tool, initiating a process in the process tool, and recording tool data for at least one observation during the process in the process tool to form a tool data matrix, where the tool data comprises a plurality of tool data parameters. The method further comprises the steps of performing a matrix multiplication of the tool data matrix and a correlation matrix to form predicted process performance data, where the correlation matrix comprises the process performance prediction model, comparing the predicted process performance data with target process performance data, and determining a fault condition of the material processing system from the comparing step.

[0010]   The present invention also advantageously provides a method for detecting a fault in a material processing system comprising the steps of recording first tool data for a plurality of observations during a first process in a process tool to form a first tool data matrix, where the first tool data comprises a plurality of tool data parameters, and recording first process performance data for the plurality of observations during the first process in the process tool to form a first process performance data matrix, where the first process performance data comprises one or more process performance parameters. The method further comprises the steps of performing a partial least squares analysis using the first tool data matrix and the first process performance data matrix, computing a correlation matrix from the partial least squares analysis, where the correlation matrix comprises a process performance prediction model, and preparing a process tool of the material processing system. The method also comprises the steps of initiating a second process in the process tool of the material

processing system, recording second tool data for at least one observation during the second

process in the process tool to form a second tool data matrix, where the second tool data

vector comprises the plurality of tool data parameters, performing a matrix multiplication of

the second tool data matrix and the correlation matrix to form predicted process performance

data, comparing the predicted process performance data with target process performance

data, and determining a fault condition of the material processing system from the comparing

step.

Brief Description of the Drawings

[0011]   These and other advantages of the invention will become more apparent and more

readily appreciated from the following detailed description of the exemplary embodiments of

the invention taken in conjunction with the accompanying drawings, where:

[0012]   Figure 1 shows a material processing system according to a preferred embodiment

of the present invention;

[0013]   Figure 2 shows a material processing system according to one embodiment of the

present invention;

[0014]   Figure 3 shows a material processing system according to another embodiment of

the present invention;

[0015]   Figure 4 shows a material processing system according to a further embodiment of

the present invention;

[0016]   Figure 5 shows a material processing system according to an additional embodiment

of the present invention;

[0017]   Figure 6 presents a schematic representation of some of the inputs and outputs for a

partial least squares (PLS) analysis model;

[0018]   Figure 7 presents an output of statistics from a PLS analysis model;

[0019]   Figure 8 presents a plot of work set loadings $w*c(1)$ versus $w*c(2)$;

[0020]   Figure 9 presents a plot of work set scores $t(1)$ versus $u(1)$;

[0021]   Figure 10 presents an exemplary set of coefficients for a mean trench etch depth model;

[0022]   Figure 11 presents an exemplary set of coefficients for a trench etch depth range model;

[0023]   Figure 12 presents an exemplary distribution for a set of variable importance in the projection (VIP) data;

[0024]   Figure 13 shows exemplary criteria for refining the tool data using VIP data;

[0025]   Figure 14 presents an exemplary comparison between the observed mean trench etch depth and the predicted mean trench etch depth;

[0026]   Figure 15 presents an exemplary comparison between the observed trench etch depth range and the predicted trench etch depth range;

[0027]   Figure 16 presents an exemplary flow diagram of a method of constructing a process performance prediction model according to an embodiment of the present invention; and

[0028]   Figure 17 presents an exemplary flow diagram of a method of fault detection using a process performance prediction model according to an embodiment of the present invention.

Detailed Description of Preferred Embodiments

[0029]   According to an embodiment of the present invention, a material processing system 1 is depicted in Figure 1 that includes a process tool 10 and a process performance prediction

system 100. The process performance prediction system 100 includes a plurality of sensors 50 and a controller 55. Alternately, the material processing system 1 can include a plurality of process tools 10. The sensors 50 are coupled to the process tool 10 to measure tool data and the controller 55 is coupled to the sensors 50 in order to receive tool data. Alternately, the controller 55 is further coupled to process tool 10. Moreover, the controller 55 is configured to predict process performance data for the process tool using the tool data. The process performance data can include at least one of a process rate and a process uniformity.

[0030] In the illustrated embodiment depicted in Figure 1, the material processing system 1 utilizes a plasma for material processing. Desirably, the material processing system 1 includes an etch chamber. Alternately, the material processing system 1 includes a photoresist coating chamber such as, for example, a photoresist spin coating system; a photoresist patterning chamber such as, for example, an ultraviolet (UV) lithography system; a dielectric coating chamber such as, for example, a spin-on-glass (SOG) or spin-on-dielectric (SOD) system; a deposition chamber such as, for example, a chemical vapor deposition (CVD) system or a physical vapor deposition (PVD) system; a rapid thermal processing (RTP) chamber such as, for example, a RTP system for thermal annealing; or a batch diffusion furnace.

[0031] According to the illustrated embodiment of the present invention depicted in Figure 2, the material processing system 1 includes process tool 10, substrate holder 20, upon which a substrate 25 to be processed is affixed, gas injection system 40, and vacuum pumping system 58. Substrate 25 can be, for example, a semiconductor substrate, a wafer, or a liquid crystal display (LCD). Process tool 10 can be, for example, configured to facilitate the generation of plasma in processing region 45 adjacent a surface of substrate 25, where plasma is formed via collisions between heated electrons and an ionizable gas. An ionizable gas or

mixture of gases is introduced via gas injection system 40, and the process pressure is adjusted. Desirably, plasma is utilized to create materials specific to a predetermined materials process, and to aid either the deposition of material to substrate 25 or the removal of material from the exposed surfaces of substrate 25. For example, controller 55 can be used to control vacuum pumping system 58 and gas injection system 40.

[0032] Substrate 25 can be, for example, transferred into and out of process tool 10 through a slot valve (not shown) and chamber feed-through (not shown) via robotic substrate transfer system where it is received by substrate lift pins (not shown) housed within substrate holder 20 and mechanically translated by devices housed therein. Once substrate 25 is received from substrate transfer system, it is lowered to an upper surface of substrate holder 20.

[0033] For example, substrate 25 can be affixed to the substrate holder 20 via an electrostatic clamping system 28. Furthermore, substrate holder 20 can further include a cooling system including a re-circulating coolant flow that receives heat from substrate holder 20 and transfers heat to a heat exchanger system (not shown), or when heating, transfers heat from the heat exchanger system. Moreover, gas can be delivered to the back-side of the substrate via a backside gas system 26 to improve the gas-gap thermal conductance between substrate 25 and substrate holder 20. Such a system can be utilized when temperature control of the substrate is required at elevated or reduced temperatures. For example, temperature control of the substrate can be useful at temperatures in excess of the steady-state temperature achieved due to a balance of the heat flux delivered to the substrate 25 from the plasma and the heat flux removed from substrate 25 by conduction to the substrate holder 20. In other embodiments, heating elements, such as resistive heating elements, or thermo-electric heaters/coolers can be included.

[0034]   As shown in Figure 2, substrate holder 20 includes an electrode through which RF power is coupled to plasma in processing region 45. For example, substrate holder 20 can be electrically biased at an RF voltage via the transmission of RF power from RF generator 30 through impedance match network 32 to substrate holder 20. The RF bias can serve to heat electrons to form and maintain plasma. In this configuration, the system can operate as a reactive ion etch (RIE) reactor, where the chamber and upper gas injection electrode serve as ground surfaces. A typical frequency for the RF bias can range from 1 MHz to 100 MHz and is preferably 13.56 MHz.

[0035]   Alternately, RF power can be applied to the substrate holder electrode at multiple frequencies. Furthermore, impedance match network 32 serves to maximize the transfer of RF power to plasma in processing chamber 10 by minimizing the reflected power. Various match network topologies (e.g., L-type, π-type, T-type, etc.) and automatic control methods can be utilized.

[0036]   With continuing reference to Figure 2, process gas can be, for example, introduced to processing region 45 through gas injection system 40. Process gas can, for example, include a mixture of gases such as argon, CF_4 and O_2, or argon, C_4F_8 and O_2 for oxide etch applications, or other chemistries such as, for example, $O_2/CO/Ar/C_4F_8$, $O_2/CO/AR/C_5F_8$, $O_2/CO/Ar/C_4F_6$, $O_2/Ar/C_4F_6$, N_2/H_2. Gas injection system 40 includes a showerhead, where process gas is supplied from a gas delivery system (not shown) to the processing region 45 through a gas injection plenum (not shown), a series of baffle plates (not shown) and a multi-orifice showerhead gas injection plate (not shown).

[0037]   Vacuum pump system 58 can, for example, include a turbo-molecular vacuum pump (TMP) capable of a pumping speed up to 5000 liters per second (and greater) and a gate valve for throttling the chamber pressure. In conventional plasma processing devices

-9-

utilized for dry plasma etch, a 1000 to 3000 liter per second TMP is generally employed. TMPs are useful for low pressure processing, typically less than 50 mTorr. At higher pressures, the TMP pumping speed falls off dramatically. For high pressure processing (i.e., greater than 100 mTorr), a mechanical booster pump and dry roughing pump can be used. Furthermore, a device for monitoring chamber pressure (not shown) is coupled to the process chamber 16. The pressure measuring device can be, for example, a Type 628B Baratron absolute capacitance manometer commercially available from MKS Instruments, Inc. (Andover, MA).

[0038]   As depicted in Figure 1, process performance prediction system 100 includes a plurality of sensors 50 coupled to process tool 10 to measure tool data and a controller 55 coupled to the sensors 50 to receive tool data. The sensors 50 can include both sensors that are intrinsic to the process tool 10 and sensors extrinsic to the process tool 10. Sensors intrinsic to process tool 10 can include those sensors pertaining to the functionality of process tool 10 such as the measurement of the Helium backside gas pressure, Helium backside flow, electrostatic clamping (ESC) voltage, ESC current, substrate holder 20 temperature (or lower electrode (LEL) temperature), coolant temperature, upper electrode (UEL) temperature, forward RF power, reflected RF power, RF self-induced DC bias, RF peak-to-peak voltage, chamber wall temperature, process gas flow rates, process gas partial pressures, chamber pressure, capacitor settings (i.e., C_1 and C_2 positions), a focus ring thickness, RF hours, focus ring RF hours, and any statistic thereof. Alternatively, sensors extrinsic to process tool 10 can include those not directly related to the functionality of process tool 10 such as a light detection device 34 for monitoring the light emitted from the plasma in processing region 45 as shown in Figure 2, or an electrical measurement device 36 for monitoring the electrical system of process tool 10 as shown in Figure 2.

[0039]   The light detection device 34 can include a detector such as a (silicon) photodiode or a photomultiplier tube (PMT) for measuring the total light intensity emitted from the plasma. The light detection device 34 can further include an optical filter such as a narrow-band interference filter. In an alternate embodiment, the light detection device 34 includes a line CCD (charge coupled device) or CID (charge injection device) array and a light dispersing device such as a grating or a prism. Additionally, light detection device 34 can include a monochromator (e.g., grating/detector system) for measuring light at a given wavelength, or a spectrometer (e.g., with a rotating grating) for measuring the light spectrum such as, for example, the device described in U.S. Patent No. 5,888,337.

[0040]   The light detection device 34 can include a high resolution OES sensor from Peak Sensor Systems. Such an OES sensor has a broad spectrum that spans the ultraviolet (UV), visible (VIS) and near infrared (NIR) light spectrums. The resolution is approximately 1.4 Angstroms, that is, the sensor is capable of collecting 5550 wavelengths from 240 to 1000 nm. The sensor is equipped with high sensitivity miniature fiber optic UV-VIS-NIR spectrometers which are, in turn, integrated with 2048 pixel linear CCD arrays.

[0041]   The spectrometers receive light transmitted through single and bundled optical fibers, where the light output from the optical fibers is dispersed across the line CCD array using a fixed grating. Similar to the configuration described above, light emitting through an optical vacuum window is focused onto the input end of the optical fibers via a convex spherical lens. Three spectrometers, each specifically tuned for a given spectral range (UV, VIS and NIR), form a sensor for a process chamber. Each spectrometer includes an independent A/D converter. And lastly, depending upon the sensor utilization, a full emission spectrum can be recorded every 0.1 to 1.0 seconds.

[0042]   The electrical measurement device 36 can include, for example, a current and/or voltage probe, a power meter, or spectrum analyzer. For example, plasma processing systems often employ RF power to form plasma, in which case, an RF transmission line, such as a coaxial cable or structure, is employed to couple RF energy to the plasma through an electrical coupling element (i.e., inductive coil, electrode, etc.). Electrical measurements using, for example, a current-voltage probe, can be exercised anywhere within the electrical (RF) circuit, such as within an RF transmission line. Furthermore, the measurement of an electrical signal, such as a time trace of voltage or current, permits the transformation of the signal into frequency space using discrete Fourier series representation (assuming a periodic signal). Thereafter, the Fourier spectrum (or for a time varying signal, the frequency spectrum) can be monitored and analyzed to characterize the state of material processing system 1. A voltage-current probe can be, for example, a device as described in detail in pending U.S. Application Serial No. 60/259,862 filed on January 8, 2001, and U.S. Patent No. 5,467,013, each of which is incorporated herein by reference in its entirety.

[0043]   In alternate embodiments, electrical measurement device 36 can include a broadband RF antenna useful for measuring a radiated RF field external to material processing system 1. A commercially available broadband RF antenna is a broadband antenna such as Antenna Research Model RAM-220 (0.1MHz to 300MHz).

[0044]   In general, the plurality of sensors 50 can include any number of sensors, intrinsic and extrinsic, which can be coupled to process tool 10 to provide tool data to the controller 55.

[0045]   Controller 55 includes a microprocessor, memory, and a digital I/O port (potentially including D/A and/or A/D converters) capable of generating control voltages sufficient to communicate and activate inputs to material processing system 1 as well as monitor outputs

from material processing system 1. As shown in Figure 2, controller 55 can be coupled to and exchange information with RF generator 30, impedance match network 32, gas injection system 40, vacuum pump system 58, backside gas delivery system 26, electrostatic clamping system 28, light detection device 34, and electrical measurement device 36. A program stored in the memory is utilized to interact with the aforementioned components of a material processing system 1 according to a stored process recipe. One example of controller 55 is a DELL PRECISION WORKSTATION 530™, available from Dell Corporation, Austin, Texas.

[0046] As shown in Figure 3, material processing system 1 can include a magnetic field system 60. For example, the magnetic field system 60 can include a stationary, or either a mechanically or electrically rotating DC magnetic field in order to potentially increase plasma density and/or improve material processing uniformity. Moreover, controller 55 can be coupled to magnetic field system 60 in order to regulate the field strength or speed of rotation.

[0047] As shown in Figure 4, the material processing system can include an upper electrode 70. For example, RF power can be coupled from RF generator 72 through impedance match network 74 to upper electrode 70. A frequency for the application of RF power to the upper electrode preferably ranges from 10 MHz to 200 MHz and is preferably 60 MHz. Additionally, a frequency for the application of power to the lower electrode can range from 0.1 MHz to 30 MHz and is preferably 2 MHz. Moreover, controller 55 can be coupled to RF generator 72 and impedance match network 74 in order to control the application of RF power to upper electrode 70.

[0048] As shown in Figure 5, the material processing system of Figure 1 can include an inductive coil 80. For example, RF power can be coupled from RF generator 82 through

impedance match network 84 to inductive coil 80, and RF power can be inductively coupled

from inductive coil 80 through dielectric window (not shown) to plasma processing region

45. A frequency for the application of RF power to the inductive coil 80 preferably ranges

from 10 MHz to 100 MHz and is preferably 13.56 MHz. Similarly, a frequency for the

application of power to the chuck electrode preferably ranges from 0.1 MHz to 30 MHz and

is preferably 13.56 MHz. In addition, a slotted Faraday shield (not shown) can be employed

to reduce capacitive coupling between the inductive coil 80 and plasma. Moreover,

controller 55 can be coupled to RF generator 82 and impedance match network 84 in order to

control the application of power to inductive coil 80. In an alternate embodiment, inductive

coil 80 can be a "spiral" coil or "pancake" coil in communication with the plasma processing

region 45 from above as in a transformer coupled plasma (TCP) reactor.

[0049]   Alternately, the plasma can be formed using electron cyclotron resonance (ECR).

In yet another embodiment, the plasma is formed from the launching of a Helicon wave. In

yet another embodiment, the plasma is formed from a propagating surface wave.

[0050]   As discussed above, the process performance prediction system 100 includes

plurality of sensors 50 and a controller 55, where the sensors 50 are coupled to process tool

10 and the controller 55 is coupled to the sensors 50 to receive tool data. The controller 55 is

further capable of executing at least one algorithm to optimize the tool data received from the

sensors 50, determine a relationship (model) between the tool data and process performance

data, and use the relationship (model) for fault detection and/or prediction.

[0051]   Table 1 presents an exemplary set of tool data, to be correlated with process performance data, including sixty-one tool data parameters.

PARAMETER	DESCRIPTION	PARAMETER	DESCRIPTION
APC	Adaptive pressure control valve setting	RF_FORWARD-S	Forward RF power, Standard deviation
HE_C_PRESS	Helium backside pressure (center), Average	C2_POSITION	Capacitor no. 2 position, Average
AR_FLOW	Argon gas flow rate, Average	ESC_CURRENT	Electrostatic clamp current, Average
PRESSURE	Chamber pressure, Average	LOWER_TEMP	LEL temperature, Average
UPPER_TEMP	UEL temperature, Average	RF_REFLECT	Reflected RF power, Average
VIP_Z	Current-voltage probe impedance, Average	VIP_PHASE	Current-voltage probe phase, Average
HE_C_FLOW-S	Helium backside flow (center), Standard deviation	APC-S	Adaptive pressure control valve setting, Standard deviation
ESC_VOLTAGE-S	Electrostatic clamp voltage, Standard deviation	HE_C_PRES-S	Helium backside pressure (center), Standard deviation
MAGNITUDE-S	Match network control signal, magnitude, Standard deviation	AR_FLOW-S	Argon gas flow rate, Standard deviation
RF_VDC-S	DC voltage, RF system, Standard deviation	PRESSURE-S	Chamber pressure, Standard deviation
VIP_RF_ON-S	Current voltage probe on/off status, Standard deviation	UPPER_TEMP-S	UEL temperature, Standard deviation
C1_POSITION	Capacitor no. 1 position, Average	VIP_Z-S	Current-voltage probe impedance, Standard deviation
HE_E_PRES	Helium backside pressure (edge), Average	HE_C_FLOW	Helium backside flow (center), Average
C5F8_FLOW	C5F8 gas flow rate, Average	ESC_VOLTAGE	Electrostatic clamp voltage, Average
RF_FORWARD	Forward RF power, Average	MAGNITUDE	Match network control signal, magnitude, Average
VIP_I	Current-voltage probe current, Average	RF_VDC	DC voltage, RF system, Average
WALL_TEMP	Chamber wall temperature, Average	VIP_RF_ON	Current voltage probe on/off status, Average
HE_E_FLOW-S	Helium backside flow (edge), Standard deviation	C1_POSITION-S	Capacitor no. 1 position, Standard deviation
O2_FLOW-S	Oxygen gas flow rate, Standard deviation	HE_E_PRES-S	Helium backside pressure (edge), Standard deviation
PHASE-S	Match network control signal, phase, Standard deviation	C5F8_FLOW-S	C5F8 gas flow rate, Standard deviation
RF_VPP-S	RF voltage peak-to-peak, Standard deviation	VIP_I-S	Current-voltage probe current, Standard deviation
VIP_V-S	Current-voltage probe voltage, Standard deviation	WALL_TEMP-S	Chamber wall temperature, Standard deviation
HE_E_FLOW	Helium backside flow (edge), Average	VIP_PHASE-S	Current-voltage probe phase, Standard deviation
O2_FLOW	Oxygen gas flow rate, Average	RF_HR	RF hours
PHASE	Match network control signal, phase, Average	SLOT_ID	Wafer slot index
RF_VPP	RF voltage peak-to-peak, Average	RF_HRxFR_THK	RF hours (X) Focus ring thickness
VIP_V	Current-voltage probe voltage, Average	RF_HRxFR_RFHR	RF hours (X) Focus ring RF hours
C2_POSITION-S	Capacitor no. 2 position, Standard deviation	FR_THK	Focus ring thickness
ESC_CURRENT-S	Electrostatic clamp current, Standard deviation	FR_RFHR	Focus ring RF hours
LOWER_TEMP-S	LEL temperature, Standard deviation	FR_THKxFR_RFHR	Focus ring thickness (X) Focus ring RF hours
RF_REFLECT-S	Reflected RF power, Standard deviation		

TABLE 1: Exemplary tool data.

[0052]   Moreover, an exemplary set of process performance data pertaining to trench etching as part of a damascene process can include a trench mean etch depth and a trench etch depth range. The mean etch depth can, for example, include a spatial average of the trench etch depth at a plurality of locations on a substrate. The trench etch depth range can, for example, include a minimum-maximum range, a variance, a standard deviation, or a root mean square (rms) of the data scatter about the mean value for the etch depth.

[0053]   The measurement of the trench etch depth and trench etch depth range can be performed directly using a scanning electron microscope (SEM) to view SEM micrographs from cleaved substrates, or indirectly using advanced, in-situ technology such as, for example, DUV spectroscopic ellipsometry (e.g., see "Specular spectroscopic scatterometry", *IEEE Transactions on Semiconductor Manufacturing*, **Vol. 14**, No. 2, May 2001) which is incorporated herein by reference in its entirety. A commercially available product featuring

optical digital profilometry (ODP) is sold and distributed by Timbre Technologies, Inc., A

TEL Company (5341 Randall Place, Fremont, CA 94538) coupled with the hardware from

Therma-Wave, Inc. (1250 Reliance Way, Fremont, CA 94539).

[0054]   Each set of data, including both tool data and corresponding process performance

data, includes an observation set, where either a single observation can be made per substrate

or a plurality of observations can be performed per substrate. Each observation in an

observation set, including both tool data and process performance data, can include an nth

order statistic (i.e., time average, rms of time trace, skewness of time trace, etc.). For

example, each observation set can correspond to a substrate processed, where each tool data

parameter is sampled during the length of the process, trimmed (i.e., data at the start and end

of the sampled data is trimmed to remove start/end transients), and averaged.

[0055]   Given a plurality of observations sets, a relationship can be determined between the

tool data in the plurality of observation sets and the process performance data in the plurality

of observation sets using multivariate analysis (MVA). One exemplary MVA technique for

determining such a relationship is partial least squares (PLS) modeling.

[0056]   Using PLS, observation sets of tool data are received from a plurality of sensors 50

and recorded using controller 55. For each observation set, tool data can be stored as a row in

a matrix $\overline{X}$ and process performance data can be stored as a row in matrix $\overline{Y}$. Hence, once

the matrix $\overline{X}$ is assembled, each row represents a different observation and each column

represents a different tool data parameter (from Table 1), and, once the matrix $\overline{Y}$ is

assembled, each row represents a different observation and each column represents a

different process performance parameter. Hence, using the set of parameters in Table 1,

matrix $\overline{X}$ is a rectangular matrix of dimensions M by sixty-one, where M is the number of

observation sets. Similarly, matrix $\overline{Y}$ is a rectangular matrix of dimensions M by two. More

generally, matrix $\overline{X}$ can be an m by n matrix, and matrix $\overline{Y}$ can be an m by p matrix. Once

all of the data is stored in the matrices, the data can be mean-centered and/or normalized, if

desired. The process of mean-centering the data stored in a matrix column involves

computing a mean value of the column elements and subtracting the mean value from each

element. Moreover, the data residing in a column of the matrix can be normalized by the

standard deviation of the data in the column.

[0057]   In the following discussion, a set of tool data and process performance data is

utilized from forty-five substrates in order to present the method by which tool data are

optimized and a model is established for relating the tool data and the process performance

data (i.e., M equals forty-five in the above discussion). The forty-five process runs

(substrates) includes three sets of substrates processed in an etch chamber, where each set of

substrates is preceded by a chamber wet clean. The tool data included in the PLS analysis

model is listed in Table 1, and the process performance data includes the mean trench etch

depth and the trench etch depth range.

[0058]   In the PLS analysis, a set of loading (or correlation) coefficients can be defined

which relate the tool data ($\overline{X}$) to the process performance data ($\overline{Y}$). In general, for

multivariate analysis, the relationship between the tool data and the process performance data

can be expressed as follows:

$$\overline{XB} = \overline{Y}\,; \qquad (1)$$

where $\overline{X}$ represents the m by n matrix described above, $\overline{B}$ represents an n by p (p<n) loading

(or correlation) matrix and $\overline{Y}$ represents the m by p matrix described above.

[0059]   Once the data matrices $\overline{X}$ and $\overline{Y}$ are assembled, a relationship designed to best

approximate the $\overline{X}$ and $\overline{Y}$ spaces and to maximize the correlation between $\overline{X}$ and $\overline{Y}$ is

established using PLS analysis.

[0060]   In the PLS analysis model, the matrices $\overline{X}$ and $\overline{Y}$ are decomposed as follows:

$$\overline{X} = \overline{TP}^T + \overline{E}; \qquad (2a)$$

$$\overline{Y} = \overline{UC}^T + \overline{F}; \qquad (2b)$$

and

$$\overline{U} = \overline{T} + \overline{H}; \qquad (2c)$$

where $\overline{T}$ is a matrix of scores that summarizes the $\overline{X}$ variables, $\overline{P}$ is a matrix of loadings for

matrix $\overline{X}$, $\overline{U}$ is a matrix of scores that summarizes the $\overline{Y}$ variables, $\overline{C}$ is a matrix of weights

expressing the correlation between $\overline{Y}$ and $\overline{T}(\overline{X})$, and $\overline{E}$, $\overline{F}$ and $\overline{H}$ are matrices of

residuals. Furthermore, in the PLS analysis model, there are additional loadings $\overline{W}$ called

weights that correlate $\overline{U}$ and $\overline{X}$, and are used to calculate $\overline{T}$. In summary, the PLS analysis

geometrically corresponds to fitting a line, plane or hyper plane to both the $\overline{X}$ and $\overline{Y}$ data

represented as points in a multidimensional space, with the objective of closely

approximating the original data tables $\overline{X}$ and $\overline{Y}$, and maximizing the covariance between the

observation positions on the hyper planes.

[0061]   Figure 6 provides a schematic representation of the data inputs, $\overline{X}$ and $\overline{Y}$, to the

PLS analysis and the corresponding outputs $\overline{T}$, $\overline{P}$, $\overline{U}$, $\overline{C}$, $\overline{W}$, $\overline{E}$, $\overline{F}$, $\overline{H}$ and variable

importance in the projection (VIP). An example of a commercially available software which

supports PLS analysis modeling is SIMCA-P 8.0. For further details on this software see the

User's Manual (User Guide to SIMCA-P 8.0: A new standard in multivariate data analysis, Umetrics AB, Version 8.0, September 1999).

[0062] In general, SIMCA-P outputs other important information regarding the descriptive power of the model (e.g., the quality of the correlation obtained between $\overline{X}$ and $\overline{Y}$), and the predictive power of the model. For example, SIMCA-P iteratively computes one PLS component at a time, that is one vector each of X-scores $\overline{T}$, Y-scores $\overline{U}$, weights $\overline{W}$ and $\overline{C}$, and loadings $\overline{P}$. The PLS components are calculated in descending order of importance. After each PLS component, SIMCA-P can display the following: the fraction of the sum of squares (SS) of all Y's and X's explained by the current component (R^2X, R^2Y); the fraction of variance of all the Y's and X's explained by the current component (R^2Xadj, R^2Yadj); the cumulative SS of all the Y's and X's explained by all extracted components ($R^2X(cum)$, $R^2Y(cum)$); and the cumulative variance of all the Y's and X's explained by all extracted components ($R^2Xadj(cum)$, $R^2Yadj(cum)$).

[0063] Furthermore, for every active variable, the fraction of SS (R^2V) or variance (R^2Vadj) explained can be displayed. This value is computed for both the current component and accumulated over all PLS components. For response variables $\overline{Y}$, this value corresponds to R^2 (the multiple correlation coefficient), the "goodness" of the fit. For example, utilizing the data above, Figure 7 presents this value for $\overline{Y}$ ($R^2VY(cum)$) for each process performance parameter, namely, the mean etch depth and the etch depth range. By inspection of Figure 7, the "goodness" of each fit exceeds ninety-seven percent when using the first four PLS components.

[0064] In general, additional criterion used to determine the model dimensionality (number of significant PLS components), is cross validation. With cross validation, observations are kept out of the model development, then the response values ($\overline{Y}$) for the kept out

observations are predicted by the model, and compared with the actual values. This procedure is repeated several times until every observation has been kept out once and only once. The prediction error sum of squares (PRESS) is the squared differences between observed $\overline{Y}$ and predicted values when the observations were kept out. For every dimension, the overall PRESS/SS is computed, where SS is the residual sum of squares of the previous dimension, and also (PRESS/SS)$_m$ for each $\overline{Y}$ variable (m). These values are good measures of the predictive power of the model, which determine a minimum number of PLS components that substantially explain a correlation between the tool data and the process performance data. For example, SIMCA-P can present this information as follows: the fraction of the total variation of the Y's that can be predicted by a component (Q^2=(1.0-PRESS/SS); the fraction of the variation of a variable Y_m that can be predicted by a component (Q^2V=(1.0-PRESS/SS)$_m$; the cumulative Q^2 for the extracted components (Q^2_{cum}=□(1.0-PRESS/SS)$_a$; and the cumulative Q^2V of a variable (Q^2V_{cum}=□(1.0-PRESS/SS)$_{ka}$). Figure 7 further presents the predictive power (Q^2V_{cum}) for each process performance parameter, namely, the mean etch depth and the etch depth range. By inspection of Figure 7, the predictive power of each fit exceeds ninety-one percent when using the first four PLS components.

[0065]   Figure 8 presents the work set loadings, w*c(1) versus w*c(2), for the tool data and process performance data described above. The plot shows both the X-weights (w or w*) and Y-weights (c), and thereby the correlation structure between $\overline{X}$ and $\overline{Y}$. One sees how the $\overline{X}$ and $\overline{Y}$ variables combine in the projections, and how the $\overline{X}$ variables relate to the $\overline{Y}$ variables. For instance, two regions (upper right hand corner and lower left hand corner) indicate where a "strong" correlation exists between the tool data parameters and the process performance parameters.

[0066]   Figure 9 presents the work set scores, t(1) versus u(1). This plot displays the objects

in the projected X(T) and Y(U) space, and shows how well the Y space coordinate (u)

correlates with the X space coordinate (t).

[0067]   Figures 10 and 11 present the coefficients assigned to each tool data parameter for

the mean etch depth model and the etch depth range model, respectively.

[0068]   Once the PLS analysis is complete and the above output matrices have been

computed, the influence on the $\overline{Y}$ matrix of every term or column in the $\overline{X}$ matrix, namely,

the VIP is determined. VIP is the sum over all model dimensions of the contributions

variable influence (VIN). For a given PLS dimension, $(VIN)_{ij}^2$ is related to the squared PLS

weight $(w_{ij})^2$ of that term. The accumulated (over all PLS dimensions) value,

$$VIP_{.j} = \sum_{i} (VIN)_{.j}^{2}, \qquad (3)$$

is used for further analysis. Once the VIPs are computed for each variable in matrix $\overline{X}$, they

may be sorted and plotted in descending order against the variable number. Those variables

with the largest VIP will have the greatest impact on the process performance data in matrix

$\overline{Y}$.

[0069]   For example, Figure 12 shows the VIP (for a four PLS component model) in

monotonically descending order; i.e., the tool data parameters falling on the left hand side of

the plot are the most significant parameters in the model.

[0070]   Using the VIP data of Figure 12, one can assess the relative significance of a given

tool data parameter on the process performance data $\overline{Y}$, and thereby refine the data matrix $\overline{X}$

by reducing the variable dimension n of the original data matrix $\overline{X}$. Exemplary criterion

used to discard the variables of minimal impact or little significance to the process

performance data include the following: (1) discard those variables whose VIP falls less than a pre-specified threshold (see Figure 13); (2) discard those variables associated with VIPs in the lowest 10th percentile or within some other predetermined range (or, in other words, retain those variables associated with the largest VIP in the top 90th percentile; note that the percentile threshold or range selected can be different from the 90/10 embodiment described herein); and (3) use the first, second or higher derivative of the VIP with respect to the variable number to select a value for the VIP, below which or above which those variables are discarded (i.e., a maximum in the first or second derivative, or when the first derivative becomes less than a predetermined threshold slope).

[0071]   Using any one of the above-mentioned criteria, one can then discard those variables that have minimal impact on the process performance data. This data reduction or refinement, in turn, reduces the column space of the data matrix $\overline{X}$ from p (sixty-one in the above example) to q (e.g., < sixty-one parameters), and forms a "new", reduced or refined data matrix $\overline{X}^{\bullet}$ of dimensions m by q (forty-five by < sixty-one). Once an initial data reduction has taken place, one may store those tool data parameters important for establishing a "good" model between the tool data and the process performance data. Thereafter, further refinement or reduction of the data matrix $\overline{X}^{\bullet}$ can be performed, and/or the method can proceed with re-computing the output matrices from the PLS analysis model using the reduced data matrix $\overline{X}^{\bullet}$ and determining the correlation matrix $\overline{B}$ for establishing the relationship between the tool data and the process performance data.

[0072]   At this point, the PLS model is repeated following the schematic presented in Figure 6, except now the reduced matrix $\overline{X}^{\bullet}$ is used as the input to the PLS analysis. The output matrices are then recomputed. As stated above, the VIPs can be studied following the

description associated with Figure 13 to further refine the data matrix $\overline{X}^{\,*}$, or the correlation

matrix $\overline{B}$ may be evaluated from the output data using the relationship:

$$\overline{B} = \overline{W} \, (\overline{P}^{\,T} \, \overline{W})^{-1} \, \overline{C}^{\,T}. \qquad (4)$$

[0073]   Once the data matrix $\overline{X}^{\,*}$ has been optimized, a final pass through the PLS analysis

is generally required to update or re-compute the output matrices necessary for computing the

correlation matrix $\overline{B}$. Hereinafter, the evaluation of equation (4) leads to a set of correlation

coefficients to be used for extracting the predicted process performance data from the

sampled tool data.

[0074]   Figure 14 presents the measured mean trench etch depth versus the predicted mean

trench etch depth, and Figure 15 presents the measured trench etch depth range versus the

predicted trench etch depth range. A slope of unity indicates a good agreement between the

measured and predicted values.

[0075]   An exemplary method for constructing a process performance prediction model

according to an embodiment of the present invention is set forth in Figure 16. Method 500

begins with step 510 where the matrix $\overline{X}$ is assembled from the observed tool data. As

described above, each column represents a different tool data parameter and each row

represents an observation. Similarly, in step 520, the matrix $\overline{Y}$ is assembled using observed

process performance data. Again, each column represents a different process performance

data parameter and each row represents an observation. In step 530, matrices $\overline{X}$ and $\overline{Y}$ are

input into the PLS analysis model to compute the above described output data (e.g., loading

data, weighting data, scores data, VIP data, etc.). (See Figures 6 through 12.) In step 540,

the PLS output statistics are checked to determine if the PLS fitting power and/or predictive

power are acceptable. In step 550, the VIP data are plotted and analyzed in descending order as in Figure 12. Using the data in step 550 from the PLS analysis, a decision whether to refine the matrix $\overline{X}$ is performed in step 560. If refinement (i.e., reduction of the number of tool data parameters to only significant tool data parameters) is required, then the procedure repeats the PLS analysis following step 570 with the new data matrix $\overline{X}^{\bullet}$ in order to re-compute the corresponding new weighting, loading, variable influence, and score matrices. In step 570, the criterion described in association with the VIP information presented in Figure 12 are utilized to reduce the matrix $\overline{X}$ to a new matrix $\overline{X}^{\bullet}$, where the reduced matrix has discarded those variables (columns) deemed unimportant for the process performance data (i.e., there is a weak correlation or minimal impact between the tool data parameter and the process performance data). Once step 560 determines that matrix $\overline{X}^{\bullet}$ is finalized, step 580 is performed. Step 580 includes computing the correlation matrix $\overline{B}$ from equation (4) for later use as a process performance prediction model. In step 590, the process performance prediction model is incorporated with, for example, a fault detection algorithm.

[0076]   Once the correlation matrix $\overline{B}$ has been evaluated (or the process performance prediction model formulated), the correlation matrix $\overline{B}$ can be used as part of a fault detection algorithm to provide robust determination and prediction of process faults. The fault detection algorithm can, in general, be applied to a variety of processes, however, the specific correlation matrix $\overline{B}$ developed as described above will be specific to a particular process in a specific process tool. For example, silicon processing, such as etching, can be performed in a process tool much like that depicted in Figures 1 through 5.

[0077]   Figure 17 presents a flow diagram of a method of detecting a fault condition for a material processing system employing a process performance prediction model according to an embodiment of the present invention. The method 600 begins with step 610 by preparing

the chamber conditions for the specific process. For example, the chamber setup includes

loading the substrate to be processed, pumping down the vacuum chamber to a base pressure,

initiating the flow of process gas, and adjusting the vacuum pump throttle valve to establish

the chamber process pressure. In step 620, the plasma is ignited via, for example, the

application of RF power to an electrode as discussed with reference to Figures 2 through 5,

thereby initiating the process. In step 630, an observation of tool data is recorded. In step

640, the established process performance prediction model is used with the observed tool data

to predict the process performance data, which includes projecting the recorded tool data onto

the one or more correlation data (process performance prediction model) via, for example,

vector multiplication (or matrix multiplication). In step 650, the predicted process

performance data are compared with target process performance data. The comparison can

include forming difference data from a numerical difference between the predicted process

performance data and the target process performance data (see Δ in Figure 13), the square of

a numerical difference, etc. In step 660, the difference data is compared with threshold

difference data, where a fault is detected and/or predicted for the process when the difference

data exceeds the threshold difference data and, conversely, the process is operating within an

acceptable range when the difference data do not exceed the threshold difference data. If the

process is operating within an acceptable range, then the process can continue in step 670. If

a fault is detected or predicted, then an operator can be notified in step 680.

[0078]   Although only certain exemplary embodiments of this invention have been

described in detail above, those skilled in the art will readily appreciate that many

modifications are possible in the exemplary embodiments without materially departing from

the novel teachings and advantages of this invention. Accordingly, all such modifications are

intended to be included within the scope of this invention.